MODELING OF HYDROGEN-AIR DIFFUSION FLAME

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Characterization of Extinction and Reignition of Hydrogen-Air Diffusion Flame

Abstract

Work performed during the first six months of the project duration for the NASA Grant (NAG-1-861) is reported here. An analytical and computational study of opposed jet diffusion flame for the purpose of understanding the effects of contaminants in the reactants and thermal diffusion of light species on extinction and reignition of diffusion flames is in progress. The methodologies that have been attempted so far are described.

Introduction

Extinction and reignition of diffusion flame are of major concern to the designers of aerospace propulsion systems. Engine reliability can be improved by knowing under what conditions extinction and reignition takes place. Velocity gradient, turbulence, presence of contaminants, and characteristics of fuel are some of the factors that affect the above mentioned phenomena. Several attempts have been made in the past to study these phenomena by experimental as well as analytical means. One commonly used experimental setup is called the opposed jet burner (Figure 1). For purposes of discussion, an axisymmetric configuration will be used here. Fuel and oxident gases, often diluted with nitrogen, flow out of axially aligned tubes of equal diameter; the two gaseous streams flow towards each other, and finally meet, creating a stagnation point flow similar to the classical stagnation point flow encountered in boundary-layer theory. Under favorable conditions, a flat diffusion flame is formed near the stagnation plane. The flame may be made to blow off or reignite in the stagnation region by changing the parameters such as flow velocity, fuel/oxident dilution level, tube diameter, and tube separation distance.

Extensive experiments have been conducted at NASA Langley Research Center on the opposed jet burner. Effects of the presence of contaminants, fuel dilution level, velocity gradient, tube size and tube separation have been extensively examined. A hysteresis phenomenon in the context of extinction and reignition, previously alluded to in the literature, has been observed and systematically documented for the first time.

Analysis and Numerical Solution

The governing equations of continuity, momentum, energy, and species continuity are transformed into a set of coupled ordinary differential equations using the boundary-layer approximations and the Howarth-Dorodnytzyn transformation. The resulting set of equations are given below.

$$(Cf_{\eta\eta})_\eta + ff_{\eta\eta} + \frac{1}{2}\left(\frac{\rho_\infty}{\rho} - f'^2\right) = 0 \tag{1}$$

$$\left(\frac{C}{Pr} h_\eta\right)_\eta + fh_\eta + \left[\frac{C}{Pr} \Sigma h_i \left\{(Le_i - 1)Y_{i\eta} + \frac{Le_i^T Y_i}{T} \frac{dT}{d\eta}\right\}\right]_\eta = 0 \tag{2}$$

$$\left(\frac{C}{Pr} Le_i Y_{i\eta}\right)_\eta + fY_{i\eta} + \left(\frac{C}{Pr} Le_i^T \frac{1}{T} \frac{dT}{d\eta}\right)_\eta + \frac{1}{2a} \frac{\dot{\omega}_i'''}{\rho} = 0 \tag{3}$$

In the above expressions $C = \rho\mu/\rho_\infty\mu_\infty$, Pr = Prandtl number, Le = Lewis number, Y = mass fraction, $\dot{\omega}'''$ = species production rate (mass/unit time/unit volume). Subscript i denotes the ith species.

The problem is thus reduced to a two-point boundary-value problem. The boundary conditions are as follows.

$$f'(-\infty) = U_{-\infty}/U_\infty = \sqrt{\rho_\infty/\rho_{-\infty}} \; ; \quad f(\infty) = 1, \quad f(0) = 0$$

$$h = \Sigma h_i Y_i; \; h(\infty) = h_{N_2} Y_{N_2} + h_{O_2} Y_{O_2} = 0 \quad (h = 0 \text{ throughout if } Le_i = 1, \; Le_i^T = 0)$$

$$h(-\infty) = h_{H_2} Y_{H_2} + h_{N_2} Y_{H_2} = 0$$

$$Y_i(-\infty) = Y_{i,-\infty} \qquad Y_i(\infty) = Y_{i,\infty}$$

Several efficient routines are available for the solution of multi-point boundary-value problems. The routine COLSYS, obtained from the mathematical library at LaRC, has been found to work well for the present problem and, therefore, it will be used for the present study.

Chemical Kinetics

The nonequilibrium nature of the flame requires chemical kinetics information for the calculation of chemical species production rates. A library of routines known as CHEMKIN, capable of generating chemical kinetics information, and thermodynamic and transport properties, has been developed at Sandia National Labs. These routines have been developed in modular form and are totally problem-independent. They have already been tested and are found to work well for the present problem. The principal investigator has already incorporated the CHEMKIN routines into the computer program developed for the present problem.

Work Completed

Numerical algorithms for the governing equations described earlier have been developed and solution attempted on the NASA Langley computer system as well as the computer system at the University of Missouri-Rolla. The following are brief descriptions of the algorithms.

1. Collocation Method: This is a routine called COLSYS [12] available from the Langley Math Library. The routine can be used to solve boundary-value problems governed by a system of ordinary differential equations.

2. Fully Implicit Finite Difference Method: Recognizing the stiff nature of the differential equations because of the presence of the chemical source term, a fully implicit algorithm was written to avoid the limitation on step size for stable solution.

3. Patankar and Spalding Method: This method uses the conservative form of the equations. The source term is treated according to the rules formulated by Patankar and Spalding [13].

Work in Progress

Rogers and Chinitz [14] global chemistry model has been used in many situations for the solution of the hydrgen-air problem. According to this model, two global reactions are used to represent the combustion of hydrogen in air. Algebraic or differential equations based on the size of the source term, are used in the numerical algorithm.

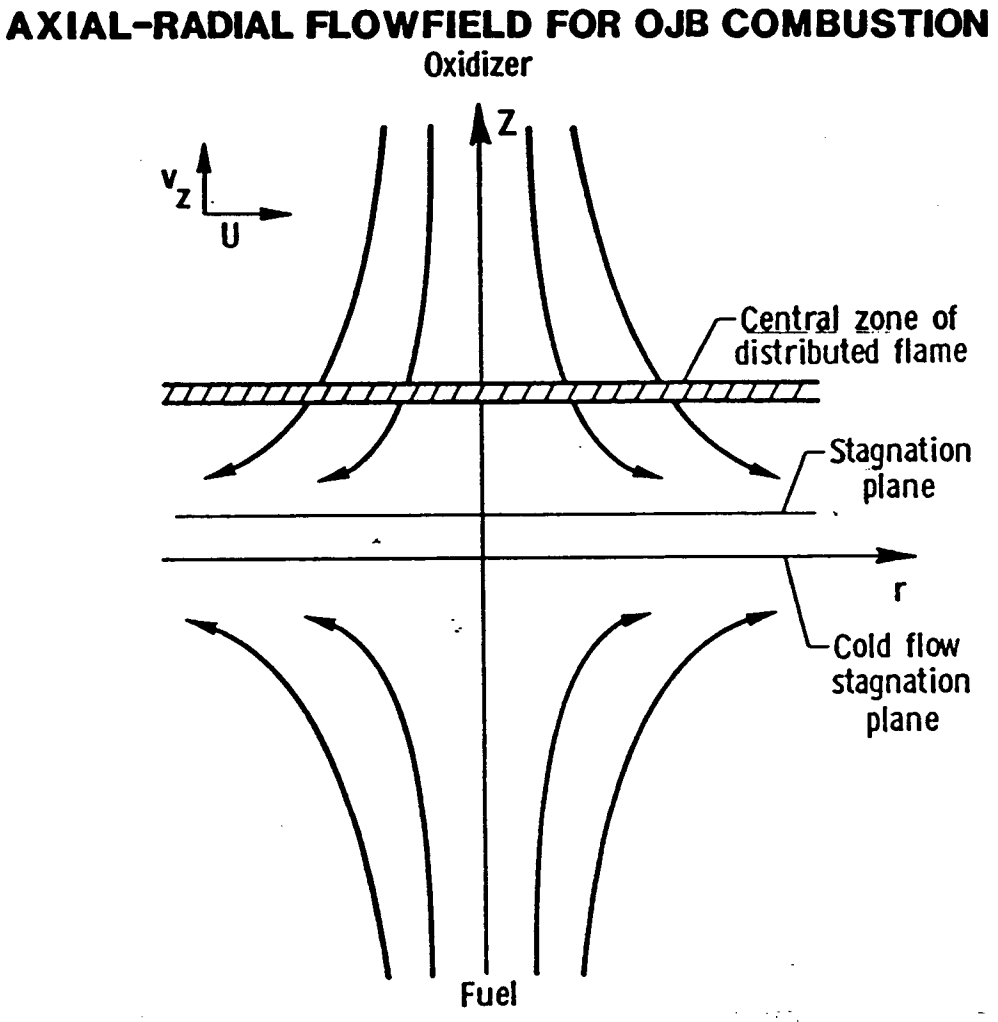

Figure 1. Illustration of the Opposed-Jet Flowfield.

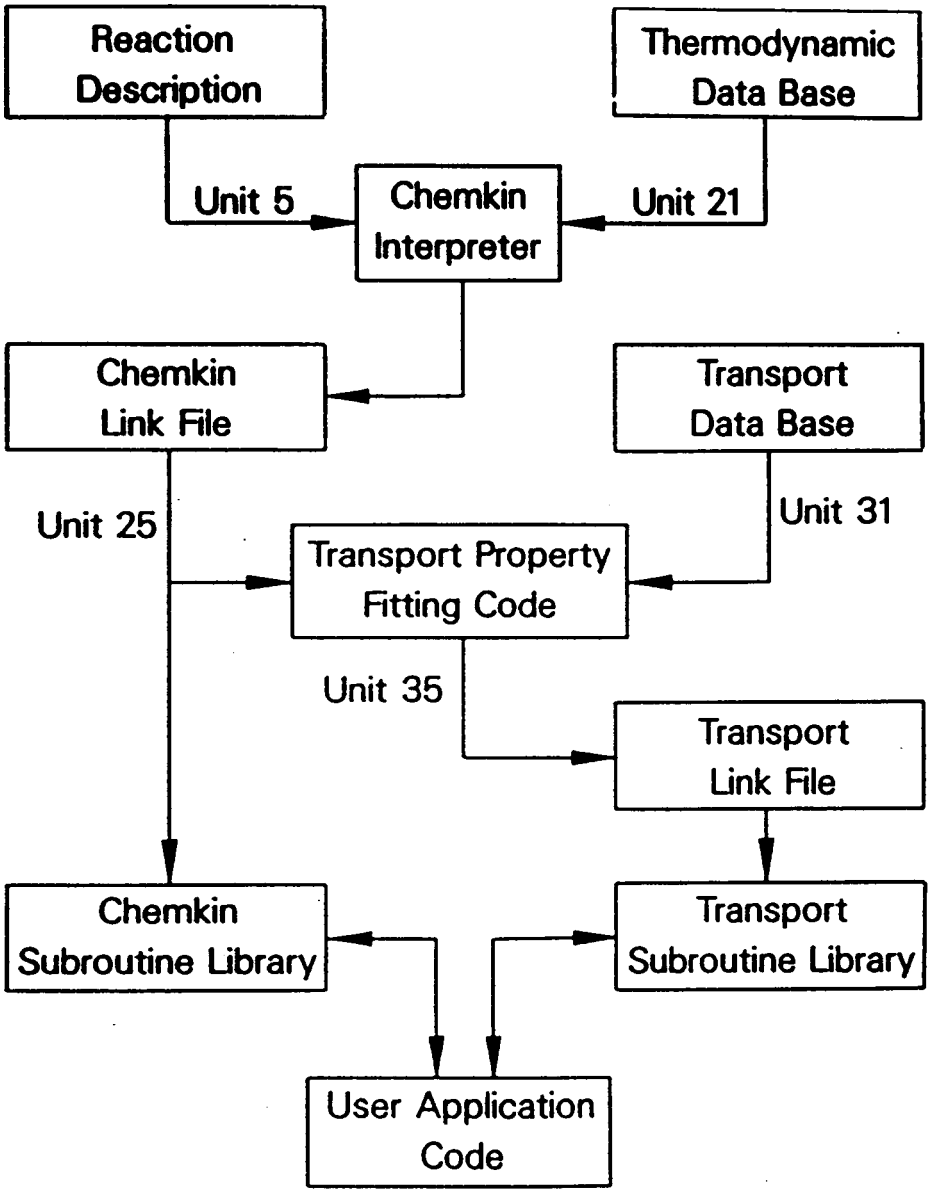

Figure 2. Program Flow Chart for Analyzing Opposed Jet Diffusion Flame.

Appendix

Thermal Diffusion Ratios

The following information is extracted from Reference 11. We consider that a thermal diffusion ratio θ_k can be defined such that the thermal diffusion velocity W_{ki} is given by

$$W_{ki} = \frac{D_k \theta_k}{X_k} \frac{1}{T} \frac{\partial T}{\partial x_i} \tag{4}$$

in which x_i is a spatial coordinate. The mole fractions are given by X_k, and the D_k are "mixture diffusion coefficients" that are defined in a following section on average properties. We only consider thermal diffusion in the trace, light component limit (specifically, species k having molecular weight less than 5). The thermal diffusion ratio is given by

$$\theta_k = \sum_{\substack{j=1 \\ j \neq k}}^{K} \theta_{kj} \tag{5}$$

in which

$$\theta_{kj} = \frac{15}{2} \frac{(2A^*_{kj} + 5)(6C^*_{kj} - 5)}{A^*_{kj}(16A^*_{kj} - 12B^*_{kj} + 55)} \frac{W_j - W_k}{W_j + W_k} X_j X_k \tag{6}$$

and

$$A^*_{kj} = \frac{\Omega^{(2,2)*}_{kj}}{\Omega^{(1,1)*}_{kj}} \tag{7}$$

$$B^*_{kj} = \frac{5\Omega^{(1,2)*}_{kj} + 4\Omega^{(1,3)*}_{kj}}{\Omega^{(1,1)*}_{kj}} \tag{8}$$

$$C^*_{kj} = \frac{\Omega^{(1,2)*}_{kj}}{\Omega^{(1,1)*}_{kj}} . \tag{9}$$

In the computer code, we store fits to A^*_{kj}, B^*_{kj}, and C^*_{kj}, instead of evaluating them from the preceeding three equations. We fit the data presented in tables by Monchick and Mason [7].

The Fitting Procedure

To expedite the evaluation of transport properties in a computer code, such as a flame code, we fit the temperature-dependent parts of the property expressions. Then, rather than evaluate the complex expressions for the properties, we need only evaluate the comparatively simple fits. The fitting procedure must be carried out for the particular system of gases that are present in a given problem. Therefore, the fitting can not be done "once and for all," but must be done once at the beginning of each new problem.

We use a polynomial fit of the logarithm of the property versus the logarithm of the temperature. For example, for the viscosity, we have

$$\ln\eta_k = \sum_{n=1}^{N} a_{n,k}(\ln T)^{n-1}, \tag{10}$$

and similarly for the thermal conductivity we have

$$\ln\lambda_k = \sum_{n=1}^{N} b_{n,k}(\ln T)^{n-1}. \tag{11}$$

The fits are done for each pair of binary diffusion coefficients in the system.

$$\ln D_{jk} = \sum_{n=1}^{N} d_{n,jk}(\ln T)^{n-1}. \tag{12}$$

The viscosities and thermal conductivities are independent of pressure, but the diffusion coefficients depend inversely on pressure. We compute all the coefficients at one atmosphere pressure. When later evaluating a diffusion coefficient, we simply divide the diffusion coefficient as evaluated from the fit by the actual pressure in atmospheres.

The thermal diffusion ratios are weakly dependent on temperature. In fitting these we use polynomials in temperature, rather than logarithm temperature. Evaluating these polynomials is more computationally efficient.

Average Mixture Properties

As the fits are done for the pure species viscosities, conductivities, and for the binary diffusion coefficients, we need a means to determine the properties of a gas mixture. We provide subroutines for the evaluation of mixture viscosities and conductivities via two different approaches.

The first approach, and the simplest, is the combination averaging formulas recommended by Mathur, et al. [8] for the evaluation of conductivity,

$$\lambda = \frac{1}{2}\left(\sum_{k=1}^{K} X_k\lambda_k + \frac{1}{\sum_{k=1}^{K} X_k/\lambda_k} \right) \tag{13}$$

in which X_k are the species mole fractions. The analogous formula for viscosity is,

$$\eta = \frac{1}{2}\left(\sum_{k=1}^{K} X_k\eta_k + \frac{1}{\sum_{k=1}^{K} X_k/\eta_k} \right) . \tag{14}$$

The semi-empirical formulas due to Wilke and modified by others can also be used to evaluate mixture properties, but they are significantly more expensive computationally, and apparently more accurate. The Wilke formulas for mixture conductivity are given by

$$\lambda = \sum_{k=1}^{K} \frac{X_k\lambda_k}{\sum_{j=1}^{K} X_j\Phi_{kj}} , \tag{15}$$

in which

$$\Phi_{kj} = \frac{1}{\sqrt{8}} \left(1 + \frac{W_k}{W_j}\right)^{-1/2} \left[1 + \left(\frac{\eta_k}{\eta_j}\right)^{1/2} \left(\frac{W_j}{W_k}\right)^{1/4} \right]^2 . \tag{16}$$

As the Φ_{kj} appears in the "inner loop", the computational expense is obvious.

There is a noticeable difference between the properties as evaluated by the two methods. At high temperature we find that the conductivities evaluated by the Wilke formulas are consistently higher (on the order of 10 percent at 2000K for hydrogen-air mixtures) than those evaluated by the combination

formulas. There is a much larger discrepancy between the two formulas for viscosities (sometimes as much as a factor of two). At least for viscosities, the Wilke formulas should be the more accurate.

We assume that a diffusion coefficient for the diffusion of species k into the gas mixture can be defined such that the species diffusion velocity is related to the mole fraction gradient in the following way:

$$\Delta_{ki} = -D_k \frac{1}{X_k} \frac{\partial X_k}{\partial x_i} . \tag{17}$$

We determine the diffusion coefficient of the species k in the mixture by the following formula:

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k}^{K} X_j / D_{jk}} \tag{18}$$

in which Y_k are the species mass fractions, and X_k the mole fractions. A potential problem with this expression is that it is not mathematically well defined in the limit of the mixture becoming a pure species. Even though diffusion itself has no real meaning in the case of a pure species, we need to be sure that in a programming implementation the diffusion coefficients behave reasonably and that the code does not "blow up" when the pure species condition is reached. We circumvent these problems by evaluating the diffusion coefficients in the following way. First, write

$$D_k = \frac{1 - Y_k}{\sum_{j \neq k}^{K} X_j / D_{jk}} = \frac{\sum_{j \neq k}^{K} Y_j}{\sum_{j \neq k}^{K} X_j / D_{jk}} , \tag{19}$$

and, as the mole fractions and mass fractions are related by

$$Y_k = \frac{X_k W_k}{W} , \tag{20}$$

we can write

$$D_k = \frac{\sum_{j \neq k}^{K} X_j W_j}{W \sum_{j \neq k}^{K} X_j / D_{jk}} . \tag{21}$$

In this form the roundoff is accumulated in roughly the same way in both the numerator and denominator, and thus the quotient is well behaved as the pure species limit is approached. However, when we have exactly a pure species, the formula is still undefined. To overcome this difficulty we add a small perturbation to the mass fractions when computing the mole fractions. In other words, for the purposes of computing mixture diffusion coefficients, we simply do not allow a pure species situation to occur; we always maintain a residual amount of each species. Specifically, we assume in the above formulas that

$$X_k = \frac{WY_k}{W_k} + \delta \ . \tag{22}$$

A value of 10^{-30} for δ works well. It is small enough that it is numerically insignificant compared to any mass fraction of interest, yet there is no trouble representing it on any computer.

Species Conservation

Some care needs to be taken in using the mixture diffusion coefficients as described here. The formulas are approximations, and they are not constrained to require that the net species diffusion flux is zero, i.e., the condition

$$\sum_{k=1}^{K} V_{ki} Y_k = 0 \tag{23}$$

is not satisfied. Therefore, one must expect that applying these mixture diffusion relationships in the solution of a system of species conservation equations should lead to some nonconservation, i.e., the resultant mass fractions will not sum to one. Therefore, one of a number of corrective actions must be invoked to ensure mass conservation.

Unfortunately, resolution of the conservation problem requires knowledge of species flux, and hence details of the specific problem and discretization

method. Therefore, it is not reasonable in the general setting to attempt to enforce conservation.

One attractive method is to define a "conservation diffusion velocity" as Coffee and Heimerl recommend. In this approach we assume that the diffusion velocity vector is given as

$$V_{ki} = \nu_{ki} + W_{ki} + V_{ci}, \tag{25}$$

in which ν_{ki} is the ordinary diffusion velocity due to mole fraction gradients, W_{ki} is the diffusion velocity due to temperature gradients, and V_{ci} is a constant correction factor (independent of species, but spatially varying) introduced to satisfy Equation 24. The correction velocity is defined by

$$V_{ci} = -\sum_{k=1}^{K} Y_k(\nu_{ki} + W_{ki}). \tag{26}$$

This approach is the one followed by Miller, et al. in their flame models.

An alternative approach is attractive in problems having one species which is always present in excess. Here, we do not solve a conservation equation for the one excess species. The excess component's mass fraction is then simply computed by subtracting the sum of the remaining mass fractions from one. A similar approach involves determining locally at each computational cell which species is in excess. The diffusion velocity for that species is computed to require satisfaction of Equation 23.

References

1. Potter, A. E. Jr. and Butler, J. N.: A Novel Combustion Measurement Based on the Extinguishment of Diffusion Flames. ARS J., Vol. 29, 1959, pp. 54-56.

2. Spalding, D. B.: Theory of Mixing and Chemical Reaction in the Opposed-Jet Diffusion Flame. ARS J., Vol. 31, 1961, pp. 763-771.

3. Fendell, F.: Ignition and Extinction in Combustion of Initially Unmixed Reactants. J. Fluid Mech., Vol. 21, Part 2, 1965, pp. 281-303.

4. Tsuji, H. and Yamaoka, I.: The Counterflow Diffusion Flame in the Forward Stagnation Region of a Porous Cylinder. 11th Symposium (International) on Combustion, The Combustion Institute, 1967, pp. 979-984.

5. Guerra, R., Pellett, G. L., Wilson, L. G., and Northam, G. B.: Opposed Jet Burner Studies of Hydrogen Combustion with Pure and N_2, NO Contaminated Air. Presented at AIAA 25th Aerospace Sciences Meeting, Jan. 12-15, 1987.

6. Pellett, G. L., Northam, G. B., Guerra, R., and Wilson, L. G.: Opposed Jet Burner Studies of Silane-Methane, Silane-Hydrogen, and Hydrogen Diffusion Flames with Air. Presented at 23rd JANNAF Combustion Meeting, Oct. 20-24, 1986.

7. Monchick, L. and Mason, E. A.: Transport Properties of Polar Gases. J. Chem. Phys., 35, p. 1676 (1961).

8. Mathur, S., Tandon, P. K., and Saxena, S. C., Thermal Conductivity of Binary, Ternary and Quaternary Mixtures of Rare Gases. Mol. Phys., 12, p. 569, 1967.

9. Wilke, C. R.: A Viscosity Equation for Gas Mixtures. J. Chem. Phys., 18, 517, 1950.

10. Coffee, T. P. and Heimerl, J. M.: Transport Algorithms for Premixed Laminar, Steady-State Flames. Comb. Flame, 43, p. 273, 1981.

11. Kee, R. J., Warnatz, J., and Miller, J. A., Sandia Report SAND83-8209, 1983.

12. Asher, U., Christiansen, J and Russell, R. D., "COLSYS: Collocation Software for Boundary-Value ODEs, ACM Trans. on Math. Software, Vol.7.

13. Patankar, S. V., Numerical Heat Transfer and Fluid Flow, Hemisphere, Washington, D.C., 1980.

14. Rogers, R. C. and Chinitz, W., "Using a Global Hydrogen-Air Combustion Model in Turbulent Reacting Flow Calculations, AIAA J, Vol.22, 1983.